On the Reprocessing and Reanalysis of Observations for Climate

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ABSTRACT

The long observational record is critical to our understanding of the Earth's climate, but most observing systems were not developed with a climate objective in mind. As a result, tremendous efforts have gone into assessing and reprocessing the data records to improve their usefulness in climate studies. Many challenges remain, such as tracking the improvement of processing algorithms and limited spatial coverage. Reanalyses have fostered significant research, yet reliable global trends in many physical fields are not yet attainable, despite significant advances in data assimilation and numerical modeling. Communication of the strengths, limitations and uncertainties of reprocessed observations and reanalysis data, not only among the community of developers, but also with the extended research community, including the new generations of researchers and the decision makers is crucial for further advancement of the observational data records. WCRP provides the means to bridge the different motivating objectives on which national efforts focus.

1 Reprocessing Observations

A major difficulty in understanding past climate change is that, with very few exceptions, the systems used to make the observations that climate scientists now rely on were not designed with their needs in mind. Early measurements were often made out of simple scientific curiosity; latterly, many systems have been driven by the needs of operational weather forecasting, or by accelerating improvements in technology. Current observation system requirements for climate monitoring and model validation such as those specified by GCOS (GOOS etc http://www.wmo.int/pages/prog/gcos/index.php?name=ClimateMonitoringPrinciples) are rarely aligned with the capabilities of historical observing systems, emphasising continuity and stability over resolution and timeliness. Nonetheless, reliable records of global temperature have been extended back to the mid nineteenth century and multidecadal series of other climatological variables now exist.

The difficulties of converting raw observations into climate-ready analyses are well documented. Inhomogeneities in data series caused by changes in instrumentation and in the environment of the sensor are often as large, or larger than, the signals we hope to detect. Without reliable traceability back to international measurement standards the problem of detecting and accounting for these inhomogeneities is not easy. Another difficulty is that before the satellite era, historical observations were often sparsely distributed. Various methods have been devised to impute the values of climatological variables at locations and times when no such observations were made.

Although many users are aware of the potential problems with observed data sets, there is a tendency to consider observations as unproblematic data points which one can use to challenge theories and hypotheses regarding the climate. In reality, the observations themselves form a system of hypotheses concerning the means by which the observed quantity is related to the climatological variable of interest. For example, satellites typically measure radiances which can be related to sea-surface temperature only by a process of modeling the atmospheric profiles and the near-surface ocean stratification. The most sophisticated examples of such systems are reanalyses, which are discussed later.

Because climate data sets derived from observations are themselves somewhat hypothetical they are open to falsification, or to competition between conflicting hypotheses. One long running example of this can be seen in the different reprocessings of the Microwave Sounding Unit (MSU) data by the University of Alabama, Huntsville (Christy et al. 2003) and Remote Sensing Systems (Mears and Wentz 2009a and 2009b) to derive vertical temperature profiles through the free atmosphere. Even after 15 or more years of analysis and reprocessing temperature trends from the different products do not agree (Thorne et al. 2010). In such cases, one might have greater confidence in conclusions that rely on features of the observations that are common to all extant data sets than in conclusions that depend on choosing one data set from many. Furthermore, it highlights the great value in having multiple analyses which span a range of underlying assumptions, the better to understand the deeper underlying uncertainties. The corollary of this is that the reliability of the data will depend very much on the application, so a one-size-fits-all approach to data set production is not feasible. The Global Precipitation Climatology Centre (GPCC) explicitly recognizes this by providing a range of data sets tailored for different uses. Information about the relative strengths, weaknesses or limitations of data sets, is often dissociated from the data themselves. Web sites such as the climate data guide (https://climatedataguide.ucar.edu/), aim to provide a central repository for expert guidance on the use of climate data sets of various kinds.

The view of competing hypotheses drives improvements in the understanding of the data and highlights the fact that no reprocessing is likely to be final and definitive. In the past decade, the view of ocean heat content has changed considerably due to the identification of time-varying biases in the measurements from eXpendable BathyThermographs (XBT). Various groups have proposed adjustments for these data based on a number of factors. By running the different correction methods on a defined set of data, it is possible to directly assess the uncertainty arising from our ignorance of the correct hypothesis (Lyman et al. 2010). A second outcome of this process is that by drawing on a broader range of hypotheses the chances of happening upon the correct hypothesis, or combination of hypotheses, are greatly improved. A similar line of reasoning can be used concerning the statistical reconstruction techniques used to impute missing values and to homogenize data. Although no statistical method can be assumed to be correct a priori, comparisons between different methods applied to carefully prepared test data sets will help to assess the relative strengths and weaknesses of the different approaches.

The International Surface Temperature Initiative (ISTI Thorne et al. 2011b) is developing a sophisticated process for developing test data sets based on synthetic 'pseudo-observations' that have been constructed to contain errors and inhomogeneities thought to be representative of real world cases. By running the algorithms designed to homogenize station data on these analogues of the real world as well as on the real data, it will be possible to directly compare the performance of different methods (e.g. Venema et al. 2012). Such processes need to be ongoing for two reasons: first benchmark tests become less useful over time because the methods become tuned to their peculiarities, second because the benchmarks might not address novel uses of the data. Such methods are less effective for assessing homogenization procedures where they are based on empirical studies (Brunet et al. 2011), or on physical reasoning (Folland and Parker

1995). However, they could be used to cross-check results if statistically-based alternatives can be developed.

A more empirical approach to the problem of assessing data biases is to run observational experiments whereby different sensors are compared side by side over a period of years. Such comparisons can be used to estimate the biases and associated uncertainties that can be used to cross check other methods, and in periods with fewer observations they may be the only means of assessing the data uncertainties.

The above concerns are vital for the creation of Climate Data Records (CDR http://www.ncdc.noaa.gov/cdr/guidelines.html), defined by the National Research Council (NRC) as "a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change". At the moment the concept of a CDR has been associated with satellite processing, but a similar approach would be illuminating for in situ measurements of other geophysical variables. Of particular interest from this point of view are the importance accorded to transparency of data and methods. Openness and transparency have many advantages over their opposites. They lay bare the assumptions made in the analysis. Although methods sections in papers can adequately describe an algorithm, there is always the danger of ambiguity, or unstated assumptions. Where computer codes are provided, they unambiguously describe the methods used. In addition, the discovery and correction of errors in data and analysis are greatly facilitated, as is the reuse of methods in later analyses.

In order to assess the sufficiency of a CDR it is necessary to understand the uncertainties associated with creating data records. Greater emphasis is now being given to the importance of observational uncertainty, but it is not always clear how a user of the data should implement or interpret published uncertainty estimates. The traditional approach of providing an error bar on a derived value is often unsatisfactory because it provides no information concerning the

covariability of errors and uncertainties in the data. Recent approaches have drawn representative samples from the posterior distributions of statistically reconstructed fields (Karspeck et al. in press) or representative samples from a particular error model (Kennedy et al. 2011). Each sample, or realization, can be run through an analysis to generate an ensemble of results that show the sensitivity of the analysis to observational uncertainty.

Assessing the quality of CDRs is a difficult task (Pirsig 1974) and uncertainty evaluations are clearly an important component of this. However, uncertainty assessments are not all equal and the data set claiming to have the narrowest uncertainty range might have grossly underestimated the uncertainties. Indices attempting to qualify the maturity of CDRs have been proposed. These include considerations of criteria such as scientific maturity, preservation maturity and metadata completeness as well highlighting the importance of independent crosschecks and the provision of validated uncertainty estimates. Validated uncertainty estimates are often difficult to produce because validation implies the availability of redundant information and a lack of data is a key problem for many observational records. For the earliest and most sparse records, physical consistency is key to elucidating and reducing the uncertainties.

An important step that remains for the understanding of historical data and hence past climate is to digitize and make freely available the vast numbers of measurements, other observations and related metadata that currently exist only in hard copy archives. Some estimates suggest that the number of undigitised marine observations prior to the Second World War is larger than the number of observations currently represented in the largest archive of surface marine observations, the International Comprehensive Ocean Atmosphere Data Set (ICOADS, Woodruff et al. 2010). Digitising large numbers of observations is labour intensive: imaging fragile paper records is time consuming and OCR technology is not yet capable of dealing with handwritten log book entries so entries must be keyed by hand.

Citizen science projects such as oldweather.org (http://www.oldweather.org) and Data.Rescue@Home (http://www.data-rescue-at-home.org/) have reliably and rapidly digitized large numbers of meteorological observations at the same time as increasing public engagement with science via lively online communities. Such projects are not only of climatological interest but can also be of wider historical interest.

With such a large range of data currently available – both raw and value added – it is difficult for users to identify, locate and obtain what they need. Planning for the needs of all users is likewise difficult, because it is not always possible to anticipate who will want to use the data or how. Other considerations are also important such as the greater need for transparency and traceability in the data and methods used. Consequently a range of possible options might be explored.

The first is to draw observational data sets together. This can occur at a variety of levels. As an example, the ICOADS draws together raw surface marine meteorological observations from many sources in a single consistent format. However, there is not as yet a systematic way to gather the value that has been added by the community that works with the ICOADS data via quality control, or bias identification and adjustment. The ICOADS does incorporate some of this information, but the IVAD (ICOADS Value Added Data) data base plans to add a layer which will give users access to a range of value-added data. No comparable comprehensive data base exists for land observations. The ISTI (International Surface Temperature Initiative) plans to create a similar archive of air temperature data and go further by planning to include full provenance information for each observation in the archive allowing users to drill down from fully analysed products to the original handwritten note made by the observer. Other projects such as Group for High Resolution Sea Surface Temperature (GHRSST, www.ghrsst.org;

Donlon et al 2007) have produced alternative models for their own user communities that give access to greater detail allowing them to make their own evaluations of uncertainty.

At a higher level there is no single repository for gridded and otherwise processed observational data sets that is analogous to the CMIP archive of model data (Meehl et al. 2000). Generating such an archive would have the dual effect of giving users easy access to the data in a standard format while allowing data producers to get their work more widely recognized. Presenting different data sets side by side will also serve to highlight the uncertainties in the observations themselves. By combining such an archive with detailed provenance information as anticipated by ISTI would allow users to use data of a kind that is appropriate for their particular analysis.

In gathering together observational data, thought must also be given to archiving and systematizing metadata and documentation. Such things as, quality flags, stations histories, calibration records, reanalysis innovations and feedback records, observer instructions, and so on, provide valuable information for analysts. Ideally archives of metadata should coexist with the archives of data to which they refer.

A problem common to all data sets is that of accurate citation. Where data sets are regularly updated, a citation to a journal paper might not be sufficient to allow full reproducibility. Data archives could allow systematic version control of data set through a common mechanism allowing future users to extract a particular data set downloaded at any time.

While these issues have been important for assessing large scale long term climate change, the challenges become even more formidable when data sets are used to assess climate change at higher resolution in time and in space. It is the extremes of weather that most often

have the highest societal impacts and detecting and attributing changes in the statistics of these events is hampered by sparse data and poorly characterised uncertainties. In order to provide the data sets demanded by climate services the problems detailed above need to be resolved for a new generation of high resolution data set - from the discovery imaging and digitising of paper records and metadata, through the management of appropriate archives, the generation of multiple independent data sets and their intercomparison to the wide dissemination and documentation of the final products.

2 Reanalysis of Observations

Reanalyses differ from reprocessed observational data sets in that sophisticated data assimilation techniques are used in combination with global forecast models to produce global estimates of continuous data fields based on multiple observational sources. One advantage of this approach is that reanalysis data products are available at all points in space and time, and that many ancillary variables, not easily or routinely observed, are generated by the forecast model subject to the constraints provided by the observations. An important disadvantage of the reanalysis technique, however, is that the effects of model biases on the reanalyzed fields depends on the strength of the observational constraint, which varies both in space and time. This needs to be taken into account when reanalysis data are used for weather and climate research (e.g. Kalnay et al 1996). Nevertheless, recent developments in data assimilation techniques, combined with improvements in models and observations (e.g. due to reprocessing of satellite data) have led to increasing use of modern reanalyses for monitoring of the global climate (Dee and Uppala 2009; Dee et al. 2011b).

With multiple reanalyses now available for weather and climate research, investigators must consider the strengths and weaknesses of each reanalysis. Estimates of the basic dynamic

fields in modern reanalyses are increasingly similar, especially in the vicinity of abundant observations. The physics fields (e.g. precipitation and longwave radiation) are more uncertain due to shortcomings in the assimilating model and its parameterizations. Understanding the effect of model errors is important both for users and developers of reanalyses, and ultimately needed to further improve the representation of climate signals in reanalysis. Observations provide the essential information content of reanalysis products; their quality and availability ultimately determines the accuracy that can be achieved. The types of observations assimilated span the breadth of remotely sensed and instrumental in-situ observations. Dealing with the complexities and uncertainties in the observing system, including data selection, quality control and bias correction, can have a crucial effect on the quality of the resulting reanalysis data.

Given the importance of reanalysis for weather and climate research and applications, successive generations of advanced reanalysis products can be anticipated. In the near future, coupling ocean, land and atmosphere will allow an integrated aspect of the reanalysis of historical observations, but may also increase the presence of model uncertainty. However, with the complexity of all the components of the Earth system, realizing the true potential of such advancements will require coordination, not only among developers of future reanalyses but also with the research community.

2.1 Current Status

The most used and cited reanalysis is the NCEP/NCAR reanalysis, which includes data going back to 1948 (Kalnay et al. 1996). The 45 year ECMWF reanalysis (ERA-40, Uppala et al. 2005), which stops in August 2002, has also been extensively used in weather and climate studies. Both of these reanalyses span the transition from a predominantly conventional observing system to the modern period with abundant satellite observations, marked by the

introduction of TOVS radiance measurements in 1979. Many spurious variations in the climate signal have been identified in these early-generation reanalyses (Bengtsson et al. 2004; Andersson et al. 2005; Chen et al. 2008a, b), mainly resulting from inadequate bias corrections of the satellite data and modulated effects of model biases related with changes in the observing system. There now exist several atmospheric reanalyses covering the post-1979 period that are being continued forward in near-real time. The Japanese 25 year Reanalysis (JRA-25), released for use in March 2006 (Onogi et al., 2007) is the first effort by the JMA, andtheir second, JRA-55 is underway (Ebita et al. 2011). The National Centers for Environmental Prediction (NCEP) second reanalysis (NCEP-DOE, Kanamitsu et al. 2002) improved upon the NCEP/NCAR reanalysis data. More recently, ECMWF has produced the ERA-Interim reanalysis based on a 2006 version of their data assimilation system (Dee et al. 2011a), in preparation for a new climate reanalysis to be produced starting in 2014. NASA's Modern Era Retrospective-analysis for Research and Applications (MERRA) was developed as a tool to better understand NASA's remote sensing data in a climate context (Rienecker et al. 2011). The NCEP Climate Forecast System Reanalysis (Saha et al. 2010) became available in early 2010, produced with a data assimilation system that includes precipitation assimilation over land, and a coupled ocean/atmosphere model.

The recent reanalyses have improved on many aspects of the earlier-generation systems. Direct assimilation of the remotely-sensed satellite radiances, rather than assimilation of retrieved state estimates, has become the norm. Variational bias correction of the satellite radiances effectively anchors these data to high-quality observations form radiosondes and other sources (Dee and Uppala, 2009; used in ERA-Interim, MERRA, and CFSR). The recently completed CFSR is the first reanalysis to use a coupled ocean/atmosphere model, and also assimilates precipitation data over land. In addition to the technical and scientific improvements

of the reanalysis systems, increased computational resources allow the use of higher-resolution models that better resolve the observations. These advances combined have lead to improved representations of many physical parameters in reanalyses, for example improved skill of the large-scale global and tropical precipitation (Bosilovich et al. 2009, 2011). In addition, the need for reanalyses to contribute to climate change studies has prompted significant innovations. For example, the 20th Century Reanalysis (20CR) project carried out by NOAA in collaboration with CIRES uses the available surface pressure observations and sea surface temperature record reconstructed through the 1870s in an ensemble-based analysis method to produce hemispheric weather patterns with the quality of a 3-day numerical forecast (Compo et al. 2011).

Even with substantial improvements, assessment of the uncertainties in reanalysis output, especially in the physical processes needed to study climate variations and change, remains a significant concern. Even the most recent reanalyses demonstrate, to varying degrees, shifts in the time series that can be related to changes in the observing systems being assimilated (Dee et al. 2011, Saha et al. 2010; Bosilovich et al. 2011). These shifts, which may be due to changing biases in the observations, systematic errors in the assimilating model, or both, interfere with the ability to detect reliable climate trends from the reanalyses. While there are some post-processing techniques that may address these spurious features (Robertson et al., 2011), dealing with biases in models and observations remains the most difficult challenge for the reanalysis and data assimilation community in developing future generations of climate reanalyses.

The number of global reanalyses has increased greatly in recent years, as computing improves, and various entities have need for specific missions to support. Furthermore, spanning the various Earth system disciplines shows that uncoupled ocean and land reanalyses are being performed as regularly as those for the atmosphere. Regional reanalyses attempt to improve upon the local representation of climate and processes that must be handled more generally in global

systems. While this increase in new and viable reanalyses can cause additional work for the research community in understanding the various strengths and weaknesses, it does provide opportunity to more quantitatively investigate the uncertainties of the reanalysis data. For example, in studying the global water and energy budgets Trenberth et al (2011) characterized the range of values for each term. In addition, collections of analyses have been used to derive a super ensemble mean and variance for the ocean (Xue et al., 2011), land (Guo et al. 2007) and atmosphere (Bosilovich et al. 2009). While the ensembles can expose biases in the character of various reanalyses, there is some evidence that the ensemble itself can also provide reasonable data from weather to monthly timescales. Despite the difficulties in dealing with a large amount of data, a researcher will find more advantage to have multiple data sets available for study. Reanalyses may well benefit from common data standards that facilitate evaluation and analysis of the IPCC climate change experiments.

2.2 Integrating Earth System Analyses

A fundamental objective of atmospheric data analysis is to provide the analyzed states to initialize numerical weather prediction. Reanalyses extend that intention to also provide a background climate to understand climate variations and anomalies. The driving force behind reanalyses are the observations, and using as many as possible to characterize the state of the Earth system. As decadal predictions begin to play a role in understanding near-term climate variations, the Earth system ocean/land/atmosphere needs to be initialized in a balanced state. Newer measurements, such as aerosols, sea ice and ocean salinity contribute to the need for reanalyses that encompass the broad Earth system. Therefore, Integrated Earth Systems Analyses (IESA) encompass the connections of these disparate observations, and have become an important challenge for data assimilation development.

NCEP CFSR provides a reanalysis produced with a coupled ocean/atmosphere model, along with an analysis of land precipitation gauge measurements (Saha et al. 2011). Development of the next reanalysis from NASA includes aerosols, ocean (temperature and salinity), land (soil water) and ocean color (biology) analysis. While there are significant difficulties in both the modeling and assimilation of the integrated Earth system, extending these more complex reanalyses to historic periods, when little or none of the diversity in observations is available will require even more effort on addressing the impact of changes in the observing systems. Likewise, maintaining and expanding many of the Earth observations forward in time is also a critical issue (Trenberth et al. OSC position paper on observing system). Consistency and overlap of newer systems will help maintain the consistency in the integrated reanalyses.

2.3 Reanalysis Observations

Essentially, reanalyses without observations revert to model data, hence the importance of the observing system emphasized here. As discussed previously, there are numerous value added advantages from reanalysis, but they cannot replace observed data products. It is very important, especially for new reanalysis users, to understand that reanalyses are not observations, but rather, an observation-based data product. Since reanalyses combine many types of observations, their relative comparison should be valuable in assessing the quality of the observation as well. However, it is not always easy to determine which observations are included in the reanalysis at specific spatio-temporal coordinates. Any given observation will be weighted against other nearby observations and the model forecast in the assimilation process. It may be accepted or rejected, and if accepted will contribute to the overall analysis including other accepted observations. The degree to which an observation influences an analysis can be determined from the output background model forecast error and the analysis error (as discussed in Rienecker et al. 2011).

Such output data have been available from reanalysis and data assimilation products for some time, but generally only used by developers or those closely familiar with the data assimilation methodology. However, these assimilated observations represent a key component in the output of the reanalyses, and can show which observations are used and how (e.g. Haimberger, 2007). To facilitate broader access, assimilated observations need to be provided in a format easily accessible to the reanalysis users, so that users can more appropriately identify the agreement between observed features (including all sources of a given state variable) and reanalysis features at any specific point in space and time. Even just the capability of easily determining the presence (or lack thereof) of assimilated observations during a given event would be useful in many research studies. Typically, the data is produced in "observations space", in that, it is an ascii record including space and time coordinates. To facilitate comparisons with the gridded reanalysis output, the GMAO has processed MERRA's assimilated observations to its native grid (Rienecker et al. 2011) called the MERRA Gridded Innovations and Observations (GIO). It includes each observation, its forecast error and analysis error (as well as the count of observations and variance within the grid box). With these data, researchers can quickly identify the most influential observation at each of the reanalysis grid points.

Of course, reanalyses rely on the broad and open availability of increasing numbers of observing systems and variables. Regarding in situ (or sometimes referred to as conventional) observing networks, reanalysis projects have been able to coordinate and update data holdings to reflect the latest quality assessments and reprocessing of the data. Some of this has been facilitated by a sub-group of the WCRP Observations and Analysis Panel (WOAP), specifically established for tracking the latest work on conventional observations regarding reanalysis projects. For the remote sensing data, however, there remains much less organization and tracking of the data used in reanalyses. As part of preparations for a new comprehensive climate

reanalysis, an inventory of satellite radiances potentially available for reanalysis is currently being compiled at ECMWF. Some remotely sensed data is still assimilated as retrieved state fields, instead of a radiance, and is therefore a function of the algorithm and its version, as well as the version of the input radiance. There is significant work progressing on the radiances themselves that should affect their use in reanalyses. For example, intercalibrated MSU (channels 2-4) (Zou et al., 2006) were newly available and assimilated from the start of MERRA production, but this was not an option for reanalyses beginning prior to it. The satellite data input is generally handled by the reanalysis center, which must maintain contacts with the data community to be informed on all the latest information and updates. Presently, each center documents its own data usage, but there is no central information about this for research users to access and intercompare among reanalyses. As discussed earlier, observations are the key resource for reanalysis, reanalysis are sensitive to the assimilated observations and so, it is vitally important for reanalysis projects to have the latest information and reprocessing of the input data type, and also convey that information to the research community.

3 Future Directions

The reanalysis developer and user community has increased substantially over the last decade, mostly due to the broad utility of the data. This paper has addressed some of the most pressing challenges facing the international reprocessing and reanalysis communities. WCRP has been an integral partner in the development of reprocessing and reanalyses, fostering communications within the community through workshops, conferences and its scientific panels. Recently, reanalyses data have been discussed and considered in the derivation of Essential Climate Variables (ECVs), as well as using the data for climate monitoring and information services (Dee et al, 2011b). Assessment of global data products is also a major issue for ECVs.

As can be easily seen in the overview summary of reanalyses, the reanalysis systems are evolving and growing. There will be newer, more advanced and comprehensive reanalysis data products available in coming years. Regarding the most recent reanalysis data products, there are many questions on their relative performance for the many uses and regions covered. It is not feasible for any one institution to be able to fully address the exact quality among all the reanalyses, simply because there are too many applications of reanalyses. While this does put the burden of intercomparison on the individual researcher, in quite a few instances, communication and sharing of knowledge between users and developers will have become critically important. In a grass roots effort to address the communications issues, an effort to utilize the internet and live documents has begun, to provide a forum that facilitates communication within the reanalysis community. It is considered a pilot project, and is called *reanalysis.org*. At this site, developers can contribute to a central knowledge-base regarding all issues of reanalyses. In the long run, users are encouraged to summarize their results with pointers to detailed information and ultimately publications on the ongoing efforts. While this should not be the sole effort to facilitate communications, it does provide an outlet and focal point for anyone in the community.

WCRP Observations and Analysis Panel (WOAP) is forming an international working group charged with coordination of reanalyses among the developing agencies. Such an entity may be able to facilitate communication among the reanalysis developers and outline best practices, but also interact with the research panels of WCRP (e.g. CLIVAR and GEWEX). It may also be able to coordinate targeted experimentation and validation, thereby addressing some user concerns on the applicability of reanalyses for certain research topics. Ultimately, the outlook for reanalyses is that they will play a significant role in many of the highest priority weather and climate research topics defined by WCRP.

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